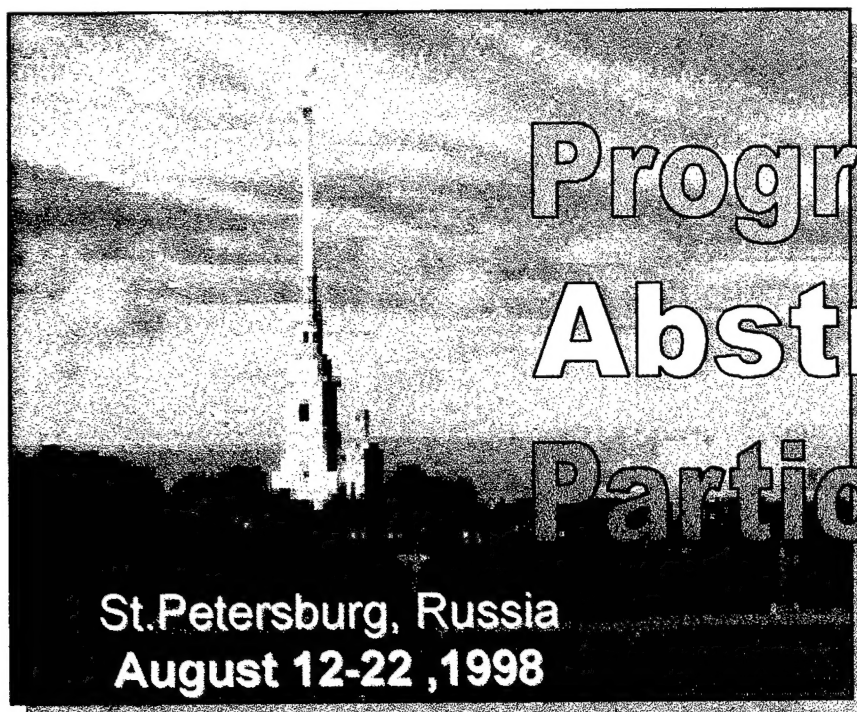


**NATO Advanced Study Institute**

# **Materials Science of Carbides, Nitrides and Borides**



**Program  
Abstracts  
Participants**

**St. Petersburg, Russia  
August 12-22, 1998**

**SPONSORED BY NATO**

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- Russian Foundation for Basic Research
- Russian Academy of Sciences, Branch of Physics and Chemistry of Inorganic Materials
- Institute for New Chemical Problems, Russia
- European Research Office of the U.S. Army
- Office of Naval Research, International Field Office, Europe
- Materials Research Center, Kiev, Ukraine
- University of Illinois at Chicago

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**NATO ADVANCED STUDY INSTITUTE**  
**MATERIALS SCIENCE of CARBIDES, NITRIDES and BORIDES**

August 12-22, 1998  
St. Petersburg, Russia

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**CONFERENCE SECRETARY:**

**A. Deriy** University of Illinois at Chicago, Department of Mechanical  
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**An Advanced Study Institute (ASI)** is a high-level teaching meeting where a carefully defined subject, systematically presented, is treated in depth by lecturers of international standing, and new advances in a field, not taught elsewhere, are reported in tutorial form. ASIs, as short courses, contribute to dissemination of knowledge and the formation of international scientific contacts. The teaching in ASIs is aimed at scientists at the postdoctoral level with an appropriate scientific background who wish to learn of recent developments.

**The objective of this ASI** is to present current research on a wide range of carbide, nitride and boride materials. Invited lecturers from the NATO, CP and other countries will present some of the most recent developments in the processing, chemistry and mechanics of these materials. Recent advances in the processing and mechanical behavior of composites in this system will be covered. Both experimental results and modeling will be discussed. We have organized a set of topic areas, which include structure and electronic properties, modeling, processing, high-temperature chemistry, oxidation and corrosion, mechanical behavior and applications of carbides, nitrides and borides.

**Expected benefits for CP countries:**

- A timely teaching forum by lecturers from NATO countries, who will review the current state-of-the-art science and technology, and address the critical issues that restrain broader applications of the materials based on carbides, borides and nitrides;
- Opportunity to meet colleagues from NATO countries and discuss possible collaboration;
- Opportunity to find potential new application for materials that were previously used only in defense;
- Access to the latest information on materials science of carbides, nitrides and borides.

**Expected benefits for NATO countries:**

- An overview of current research activities in CP countries;
- Opportunity to pursue fruitful discussions and initiate collaboration with colleagues from CP countries;
- Opportunity to meet leading scientist from the former Soviet Union;
- Opportunity to identify potential students and post-docs;
- The proceedings volume, which will be useful as a timely reference book.

**Official Language**

English (there will be NO simultaneous translation).

**Paper Preparation and Presentation**

Papers have been scheduled as invited lectures (1 hour + 30 min discussion), short talks (20 min) and poster presentations. All papers and/or posters must be presented in English. Care in the preparation of your oral and or/poster presentation will result in a better understanding of your work. Contact your session Chairmen if you have any questions. Your Chairmen's names appear in the ASI Program and their addresses are on the list of participants. It is advisable to introduce yourself to the Session Chairmen before the session begins.



## **Poster Preparation**

Attendees are afforded a truly unique opportunity to discuss leading-edge research one-on-one with the involved researchers. About 80 posters will be presented at the conference. Posters have been divided into three one-day sessions. Check the program for the date of your poster session. Plan your display to fit within 92 cm x 92 cm panel. Two panels can be available for extra large posters. Pins or thumbtacks will be provided. The paper title, names of the authors and their affiliations must be at the top of the display. Authors should minimize the written text. All text, illustrations, drawings, charts, pictures and graphs should be sufficiently large to allow easy reading from a distance of 1 m. Authors must be present during the entire Poster Session. Mount your posters at 8:00-9:00 a.m. and remove them at the end of the day.

## **Proceedings**

The proceedings volume from this NATO ASI will include tutorial papers. It will be published after the meeting by Kluwer in NATO ASI series. Submitted papers can be published in one of the following journals:

*Journal of Materials Processing and Manufacturing Science* (in English)

*Advances in Technology of Materials and Processing Journal* (ATM) (in English)

*Ogneupory i Tekhnicheskaya Keramika* (in Russian, with English translation)

Please choose a journal according to the topic and the language of your paper. It is important that you follow the rules and standards of the journals. All manuscripts are due on the first day of the conference.

## **Registration Fees**

Conference registration is free for all invited attendees from academic and research institutions in NATO and CP countries. It includes sessions, program/abstracts, proceedings (1 book per institution), welcome reception, social activities, coffee breaks and airport transportation. Attendees from industry and from other countries, as well as accompanying guests, are required to pay a small registration fee, unless waived by ASI directors. The conference fee includes sessions, proceedings, welcome reception, banquet, social activities, coffee breaks and airport transportation.

### Conference Registration Fee is:

- US \$ 200.00 - participants from industry (NATO countries).
- US \$ 50.00 – participants from industry (CP countries, banquet is not included).
- US \$ 300.00 – participants from other countries.
- US \$ 50 - accompanying person (includes welcome reception, banquet and other social events. Access to sessions, transportation and tours are not included).
- Additional reception tickets - \$ 20.
- Banquet tickets - \$ 27.
- Domestic airport transportation - \$ 5 each way.
- International airport transportation - \$ 10 each way.

Tour and excursion tickets are not included in the registration and must be purchased at the conference desk.

### **Accommodation**

For convenience of the participants, the primary accommodation will be provided at the State Education Center (SEC) of St. Petersburg. It is located in 5 to 10 minutes walking from metro station "Pionerskaya".

#### Address:

Aerodromnaya St. 4  
St. Petersburg 197348  
RUSSIA

Contact Mr. A. Kozlov (Deputy Manager, SEC):

Phone: (812)-394-5006

Fax: (812)-394-5005

*The State Education Center (SEC)* is a traditional place for international meetings in St. Petersburg. In 1997, the SEC hosted about 40 international conferences and seminars.

Living expenses at SEC are about US\$ 55.00/day (single or double room, all meals included). Breakfast (\$2), lunch (\$12) and dinner (\$11) can be purchased separately at the SEC restaurant. Cost of accommodation in a single room is \$30/night (light breakfast is included). Stay in a double room will cost \$ 15 per night per person. Several suites are available at a higher rate (\$60-80).

### **Accompanying Guests**

Spouses and guests of ASI attendees are invited to meet and enjoy refreshments at the Welcome Reception on August 12. Information on special activities (excursions, shopping tours, etc.) for the guests will be available at the conference desk. Reception and conference dinner are included in the Conference Registration fee of \$ 50.

### **Weather**

The weather in St. Petersburg in August is moderate, with an average daytime temperature of 20°C and nighttime temperature of 14°C.

### **Sightseeing and Cultural Activities**

St. Petersburg (about 5,000,000 inhabitants) is one of the most beautiful cities in the world. There are many famous architectural ensembles, museums, theaters and concert halls in St. Petersburg. Organized excursions to museums and historical sites, and cultural activities will be planned. A bus tour of St. Petersburg and tours to Hermitage and Petrodvorets have been prearranged. Examples of other tours follow:

1. Folk show. Tradition Russian singing and dancing in a luxurious interior of the residence of Russians monarchs.

Price: \$20 including buffet with a caviar.

Time: Every night at 6:30 p.m.

2. Classical ballet of Mariinsky (Kirov) theater, one of the two leading theaters in Russia, will appear on the stage of Hermitage Theater.

Price: \$45.

Dates: Aug. 17, Aug. 19, Aug. 21.

3. Guided tour to the town of Pushkin, one of the most charming estates in vicinity of St. Petersburg. You will see Catherine's Palace and a beautiful Park. Tentative Price: \$20.

4. Excursion to Peter and Paul Fortress. The spot from which St. Petersburg began to grow and the historical center of the city. Visit Cathedral of St. Peter and St. Paul, almost all Russian tsars were buried there, including the family of the last tsar Nicholas II. Tentative Price: \$15.

5. State Russian Museum which is a treasure house of Russian art. Tentative Price: \$18

Ask at the conference desk for information on other tours.

### **Liability and Insurance**

The organizing committee feels important to inform the participants that NATO does not take out any health or accident insurance for the participation in the meeting. Such insurance is an individual responsibility. NATO does not assume any responsibility, either in this context or for any other liability.

### **Contacts**

#### Transportation and Sightseeing:

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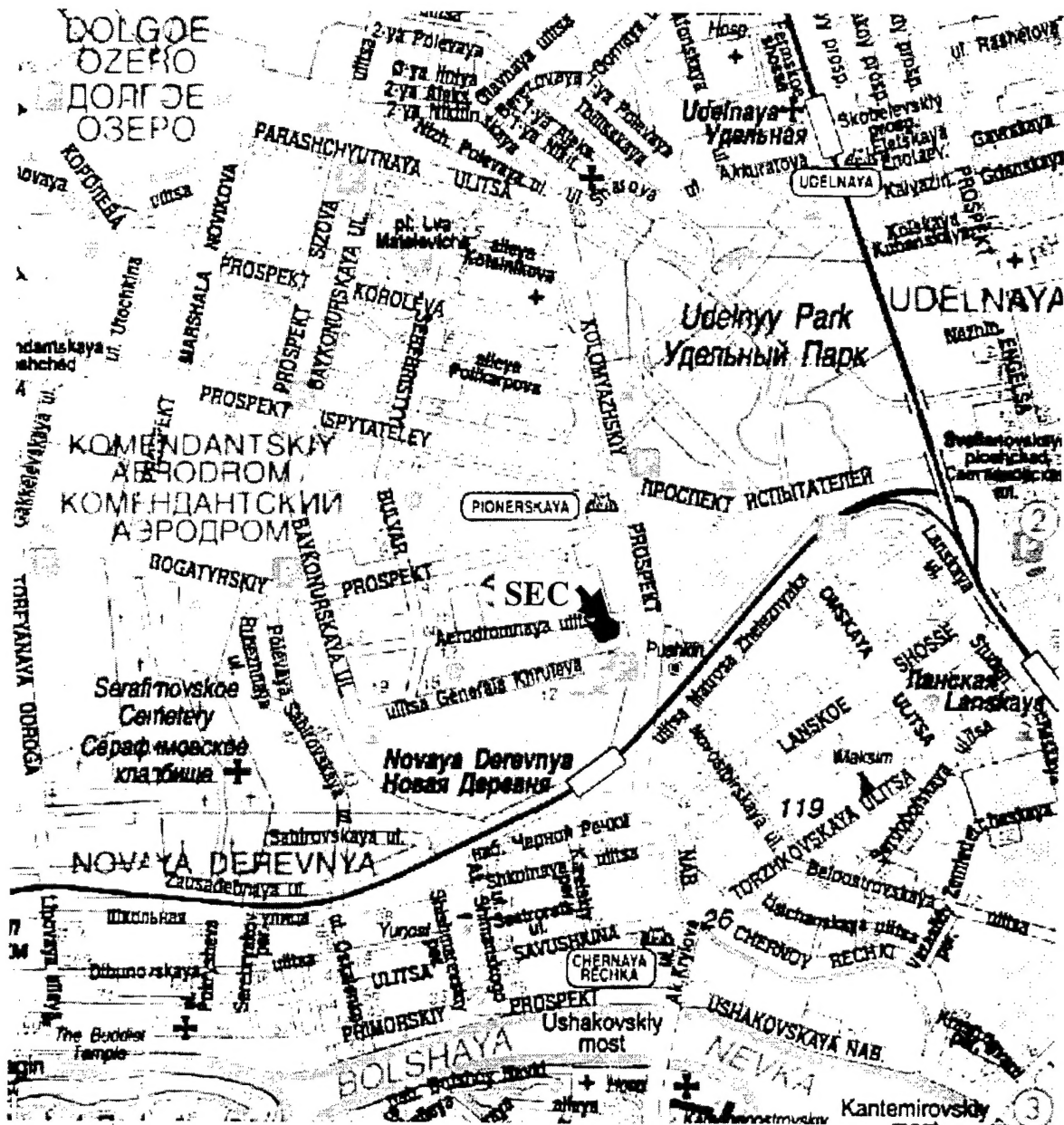
NATO ASI World Wide Web site will be updated continuously.  
Go to this address for the most up-to-date information about the conference:  
**[http://www.me.uic.edu/NATO\\_ASI.htm](http://www.me.uic.edu/NATO_ASI.htm)**

#### Webmaster:

Mr. V. Domnich  
e-mail: vdomni1@uic.edu

## ASI Location

The ASI will be held in the State Education Center (SEC) of St. Petersburg, Aerodromnaya St. 4, St. Petersburg 197348. It takes approximately 1 hour by car or bus from Pulkovo and Pulkovo-2 airports to the State Education Center. Railroad stations are about 20-40 minutes from the SEC by car. Bus transfer from airports will be organized for registered participants. SEC can be also accessed from railway stations and airports by taxi or metro. SEC is in a walking distance from the metro station “Pionerskaya”.



# TIME TABLE

Time Date	8:00-9:00	9:00-10:30	10:30-11:00	11:00-12:30	12:30-14:00	14:00-15:30	15:30-16:00	16:00-17:30	17:30-18:00	18:00-19:00
August 12 Wednesday			Arrival				Registration		Welcome Reception	
August 13 Thursday	Breakfast	<i>Andrievski</i>	Coffee break	<i>Kerch</i>	Lunch	<i>Werheit</i>	Coffee break	<i>Gusev</i>	Dinner	Bus tour
August 14 Friday	Breakfast	<i>Baraton</i>	Coffee break	<i>Trenary</i>	Lunch	<i>Sheka</i>	Coffee break	<i>Frenklach</i>	Discussion	Dinner
August 15 Saturday	Breakfast	<i>Rogl</i>	Coffee break	<i>Ovid'ko</i>	Lunch	<i>Rogl</i>	Coffee break	<i>Rogl</i>		Dinner
August 16 Sunday	Breakfast	Petrodvorets					Project meetings		Dinner	
August 17 Monday	Breakfast	<i>Sharivker</i>	Coffee break	Short papers	Lunch	<i>Paderno</i>	Coffee break	<i>Desmaison</i>	Posters I	Dinner
August 18 Tuesday	Breakfast	<i>Kuznetsov</i>	Coffee break	<i>Güçeri</i>	Lunch	<i>Bellosi</i>	Coffee break	Posters II	Discussion	Dinner
August 19 Wednesday	Breakfast	<i>Barnett</i>	Coffee break	<i>Millman</i>	Lunch	Short papers	Coffee break	Posters III	Discussion	Dinner
August 20 Thursday	Breakfast	<i>Gogotsi</i>	Coffee break	Short papers	Lunch	<i>Lavrenko</i>	Coffee break	<i>McNallan</i>	Discussion	Conference Dinner
August 21 Friday	Breakfast	<i>Lanin</i>	Coffee break	<i>Fedik</i>	Lunch	Short papers	Coffee break	Round Table	Discussion	Dinner
August 22 Saturday	Breakfast	Excursions			Departure					

## CONFERENCE PROGRAM

**Wednesday, August 12, 1998**

p.m.                    Registration  
                         Meeting of the Organizing Committee  
                         Welcome Reception

**Thursday, August 13, 1998**

a.m.                    Session I: Introductory

Chairs:                L-1  
*Y.G. Gogotsi*           "State-of-the-Art of High-Melting Compounds"  
*S. Barnett*            *R.A. Andrievski*  
                         Institute for New Chemical Problems, Russia

                         L-2  
                         "Basic Materials Research in the U.S. Department of Energy"  
                         *H. Kerch*  
                         U.S. Department of Energy, U.S.A.

p.m.                    Session II: Structure and Electronic Properties

Chairs:                L-3  
*I. Ovid'ko*            "On the Electronic Properties of Icosahedral Boron-Rich Solids"  
*M.Yu. Gutkin*        *H. Werheit*  
                         Gerhard Mercator University, Germany

                         L-4  
                         "Atomic Ordering and Phase Equilibria in Strongly Nonstoichiometric  
                         Carbides and Nitrides"  
                         *A.I. Gusev* and *A.A. Rempel*  
                         Institute of Solid State Chemistry, Russia

Evening                St. Petersburg by bus

**Friday, August 14, 1998**

a.m.

Session III: Material Surfaces

Chairs:

*I.Yu. Archakov*

*H. Werheit*

L-5

"Surface Characterization of High-Melting Point Compounds"

*M.I. Baraton*

LMCTS ESA 6015 CNRS

L-6

"Surface Structure and Chemistry of Boron-Rich Solids"

*M. Trenary*

University of Illinois at Chicago, U.S.A.

p.m.

Session IV: Modeling I

Chairs:

*L. Mehrari*

*V. Kamysenko*

L-7

"Computational Modeling of Surface Layers of Refractory Compounds"

*E.F. Sheka*

Russian Peoples Friendship University, Russia

L-8

"Numerical Modeling of Surface Reactions"

*M. Frenklach*

University of California at Berkeley, U.S.A.



**Saturday, August 15, 1998**

a.m.

Session V: Modeling II

Chairs:

*M.-J. Baraton*  
*M. Frenklach*

L-9

"Ternary Metal Boron Carbides: Constitution, Thermodynamics,  
Compound Formation and Structural Chemistry"

*P. Rogl*

University of Vienna, Austria

L-10

"Interfaces in Ceramics"

*I.A. Ovid'ko*

Institute of Machine Science Problems, Russia

p.m.

Session VI: Phase Diagrams Workshop

Chair:

*R.A. Andrievski*

"How to Read and Construct Ternary Phase Diagrams"

*P. Rogl*

University of Vienna, Austria

**Sunday, August 16, 1998**

Whole day

Petrodvorets

Group (project) meetings

**Monday, August 17, 1998**

a.m.

Session VII: Synthesis I

Chairs:

*V. Zymla*

*I.V. Uvarova*

L-11

"Self-Propagating High-Temperature Synthesis of Carbides, Nitrides and Borides"

*A.G. Merzhanov, S.Yu. Sharivker*

Institute of Structural Macro-Kinetics, Russia

Short talks:

S-1

"Combustion Synthesis of Aluminum Nitride"

*A. Zymla, V. Zymla*

Ecole Centrale Paris, France

S-2

"Plasma-Chemical Synthesis of High-Melting Nitrides"

*V.N. Troitskiy*

Institute for New Chemical Problems, Russia

S-3

"Colloidal and Aerosol Processing of Non-oxide and Composite Materials"

*D.P. Uskokovich*

Institute of Technical Sciences, Yugoslavia

S-4

"In-situ Synthesis of Silicon Carbide-Silicon Nitride Composites from Polymeric Precursors"

*M.J. Edirisinghe*

Loughborough University, U.K.

p.m.

Session VIII: Synthesis II

Chairs:

*M. Trenary*

*P. Rogl*

L-12

"Synthesis, Physical and Chemical Properties of Rare Earth Borides"

*Yu.B. Paderno, V.N. Paderno*

Institute for Problems of Materials Science, Ukraine

L-13

"Boride/Nitride Composites: Synthesis and Properties"

*J. Desmaison, M. Desmaison*

LMCTS, France

Poster Session I (Chair: *A.I. Gusev*)

**Tuesday, August 18, 1998**

a.m.

**Session IX: Materials from Polymeric Precursors**

Chairs:

*M. Edirisinghe*  
*D.P. Uskokovich*

L-14

"Physicochemistry of Precursors for Carbide, Nitride, and Boride Synthesis"

*N.T. Kuznetsov*

Institute of General and Inorganic Chemistry, Russia

L-15

"Ceramic Matrix Composites from Polymerorganic Precursors"

*S. Güçeri*

University of Illinois at Chicago, U.S.A.

p.m.

**Session X: Ceramic Technology**

Chairs:

*S. Güçeri*  
*M. Desmaison*

L-16

"Influence of Powder Treatment Methods and Additives on Sintering, Microstructure and Properties of Nonoxide Ceramics"

*A. Bellosi*

Research Institute for Ceramics Technology, Italy

**Poster Session II** (Chair: *Yu.V. Mil'man*)

**Wednesday, August 19, 1998**

a.m.

Session XI: Mechanical Behavior

Chairs:

*J. Schneider*  
*O.N. Grigoriev*

L-17

"Deposition, Structure, and Mechanical Properties of Nitride-Based Superlattices"

*S.A. Barnett*

Northwestern University, U.S.A.

L-18

"Physics of Hardness of High-Melting Compounds"

*Yu. V. Mil'man*

Institute for Problems of Materials Science, Ukraine

p.m.

Short talks:

Chair:

*A.G. Lanin*

S-5

"Correlation between Deformation Mechanisms and Microstructural Evolution in Silicon Nitride Ceramics"

*J.A. Schneider*<sup>1</sup>, *A.K. Mukherjee*<sup>2</sup>

<sup>1</sup>Sandia National Labs, USA

<sup>2</sup>University of California, USA

S-6

"Fracture Toughness of Ceramic Materials: SEVNB Method"

*G.A. Gogotsi*

Institute for Problems of Strength, Ukraine

Poster Session III (Chair: *S.Yu. Sharivker*)

Thursday, August 20, 1998

a.m.

Session XII: High-Temperature Behavior

Chairs:

M.J. McNallan

V.A. Lavrenko

L-19

"Formation of Carbon upon Selective Etching and Decomposition of Carbides"

Y.G. Gogotsi

University of Illinois at Chicago, U.S.A.

Short talks:

S-7

"Oxidation Behavior of Silicon Nitride Ceramics by *Post-mortem* and *In-situ* Observations"

V. Guerin, M. Backhaus-Ricoult

Centre d'Etudes de Chimie Metallurgique - CNRS, France

S-8

"The Influence of Surface Dynamics on the Hot Corrosion of Silica and Silica Formers"

Ch. Berthold, K.G. Nickel

Eberhard-Karls University of Tübingen, Germany

S-9

"Oxidation Behavior of Precursor Derived Ceramics in the System Si-(B)-N-C"

E. Butchereit, K.G. Nickel

Eberhard-Karls University of Tübingen, Germany

S-10

"Theoretical Investigation of Carbon Layers Structure at the Surface of Carbides"

V.V. Kamysenko, V.I. Shevchenko

Institute for Problems of Materials Science, Ukraine

p.m.

Session XIII: Corrosion

Chairs:

Ch. Berthold

J. Desmaison

L-20

"Interaction of Carbides and Nitrides with Halogen-Containing Compounds"

M.J. McNallan

University of Illinois at Chicago, U.S.A.

L-21

"Interaction of High-Melting Compounds with Aggressive Media"

V.A. Lavrenko, A.D. Panasyuk

Institute for Problems of Materials Science, Ukraine

Conference Dinner

**Friday, August 21, 1998**

a.m.                      Session XIII: Structural Ceramics

Chair:                      L-22  
                                "Strength and Thermal Shock Resistance of Refractory Compounds"  
*A. Bellosi*                      *A.G. Lanin*  
                                Scientific Industrial Association "Lutch", Russia

                                L-23  
                                "High-Temperature Structural Carbide Components"  
                                *I.I. Fedik*  
                                Scientific Industrial Association "Lutch", Russia

p.m.                      Short talks

Chair:                      S-11  
*R.A. Andrievski*                      "Effect of Vacancies on Structure and Properties of Strongly  
                                Nonstoichiometric Carbides"  
                                *A.A. Rempel*  
                                Institute of Solid State Chemistry, Russia

                                S-12  
                                "Nucleation under Heterogenous and Solid State Reactions"  
                                *I.V. Uvarova*  
                                Institute for Problems of Materials Science, Ukraine

                                S-13  
                                "Mass-spectrometric study of evaporation of heat resistive coating  
                                containing borides and silicides"  
                                *I.Yu. Archakov, S.I. Shornikov, M.M. Shultz*  
                                Institute of Silicate Chemistry, RAS, Russia

Round Table Discussion:

                                "Future Avenues of Research and Potential Applications of Carbides,  
                                Nitrides and Borides"  
                                Moderators: *I. Ovid'ko, A. Rempel, H. Werheit*

Closing remarks: (*R.A. Andrievski*)

**Saturday, August 22, 1998**

a.m.                      Excursions

## ABSTRACTS of LECTURES

L-1

### **State-of-the-Art of High-Melting Compounds**

R.A.Andrievski

*Institute for New Chemical Problems  
Russian Academy of Sciences  
Moscow, Russia*

High-melting point compounds (HMPCs) such as carbides, nitrides, and borides are the base of many advanced materials for the new millennium. Some historical essay of materials science of these compounds is presented. The outstanding role of G.V. Samsonov in the development of this scientific direction is pointed out.

Special attention is devoted to some new features of HMPCs materials science such as engineering ceramics, nanostructured materials including films, superplastic and superhard materials, interfaces, modelling, etc. As an example we refer to silicon carbide and silicon nitride which are considered to be HMPCs with the extraordinary combination of physical, chemical, and mechanical properties for many comprehensive applications.



**Basic Materials Research in the U.S. Department of Energy**

Helen Kerch

*Division of Materials Science ER-13  
US Department of Energy  
19901 Germantown Rd.  
Germantown, Maryland 20874-1290, U.S.A.*

Materials research plays a central role in underpinning key mission areas in the U.S. Department of Energy. The DOE is one of the largest federal funders of basic materials research supporting individual investigators at universities, multidisciplinary teams at DOE national labs, and research partnerships with industry. The DOE also has stewardship for 18 national user facilities including x-ray, neutron and electron microbeam characterization facilities. Strategic materials areas that advance the science and technology foundation to achieve efficiency in energy use, safe and reliable energy sources, improved environmental quality, and a fundamental understanding of matter and energy will be discussed.

## On The Electronic Properties of Icosahedral Boron-Rich Solids

Helmut Werheit

*Solid State Physics Laboratory  
Gerhard Mercator University Duisburg  
D 47048 Duisburg, Germany*

Outstanding properties of the boron-rich solids in general are their high melting temperatures, extraordinary hardness, small extension coefficients and high chemical resistivity, which predestine them for technical application at conditions which are hardly accessible for most other materials. The aim of this paper is to describe the interrelation of structural and electronic properties and to point to the potential possibilities of their modification to tailor boron-rich solids for specific, particularly electronic applications

The complex structures of different modifications of elementary boron and boron-rich borides are essentially composed of B<sub>12</sub> icosahedra and of related structural elements forming a large variety of open frameworks. The icosahedra has common structural features that are the reason for the more or less close relationships of the properties and distinguish the boron-rich solids qualitatively from crystals with periodic arrangements of single atoms.

The boron-rich solids are semiconductors with unique electronic properties essentially determined by the icosahedra. This implies an interrelation of these properties, which can be modified within the large homogeneity ranges of chemical compositions by forming ternary compounds, changing the chemical composition within the specific structure groups and going to the different structure groups.

Accordingly the icosahedral boron-rich solids offer an excellent chance to study the electronic properties of complex structures and their modification by slight and considerable changes of composition and structure. Some peculiarities of these properties with particular interest for fundamental research are the Jahn-Teller effect in the icosahedra, the formation of intrinsic traps by electron-phonon interaction, and the soliton-type transport of electrons and holes. Also of interest are the very long lifetime of electrons at specific conditions, the electronic interaction between foreign atoms and the boron framework, and the high, up to very high temperatures monotonously increasing Seebeck coefficient of boron carbide.

The specific electronic structures make the boron-rich solids insensitive against influences of foreign atoms in concentrations. This will change the semiconductor properties of classical semiconductors significantly. Nevertheless, doping is possible in principle, at higher concentration levels. This makes material preparation much easier and less expensive than classical semiconductors which demand extremely high purity.

**Atomic Ordering and Phase Equilibria  
in Strongly Nonstoichiometric Carbides and Nitrides**

A.I. Gusev and A.A. Rempel

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Ordering of the interstitial atoms (X) and structural vacancies (unfilled sites of a nonmetallic sublattice) in the strongly nonstoichiometric interstitial compounds  $MX_y$  (such as cubic and hexagonal carbides and nitrides of the transition metals) is widespread and has been currently found to occur in most of these compounds. However, ordering comes about at a temperature below 1300 K and therefore little is known about the kind of the ordered phases existing under the equilibrium conditions in the low-temperature region of M-C and M-N phase diagrams. In the present work the data on phase equilibria in M-C and M-N systems have been considered and summarized and phase diagrams of Ti-C, Zr-C, Hf-C, Nb-C, Ta-C, Ti-N systems have been constructed allowing for the ordering of nonstoichiometric carbides and nitrides that form in these systems.

## Surface Characterization of High-Melting Point Compounds

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The tremendous problem with non-oxide (carbide and nitride) materials is the hydrolysis of their surface when they are stored under atmosphere. Indeed, the combined actions of oxygen and humidity cause drastic changes in the surface ceramic layer. In the case of powders, depending on the average grain size, the oxidation process can drastically damage the non-oxide materials and destroy their specific properties. For example, it is obvious that careless sintering of nitride or carbide powders will cause oxygen incorporation in the grain boundaries ruining the properties of the consolidated material. It must also be realized that the hydrolysis and oxidation processes will depend on the surface reactivity of the nanoparticle and thus, on the surface species. Since these surface species are partly related to the synthesis parameters, it is easy to understand that the resistance to oxidation of a particular compound will depend on the synthesis route. But, on the other hand, it cannot *a priori* be considered that the surface of the nitride and carbide particles is entirely covered with an oxide layer.

The surface hydrolysis is particularly disastrous for nanosized powders as it ruins their extraordinary properties. Because of the high specific surface area of these nanoparticles, the control of the surface becomes a stringent requirement, although very few experimental techniques can analyze the first atomic layer of the particle. Indeed, most of the so-called surface techniques actually have a resolution depth comparable to the size of the particle. Of interest is Fourier transform infrared (FTIR) spectrometry which, under specific experimental conditions, is a performant tool to characterize the very first atomic layer of nanoparticles and to follow *in situ* the chemical reactions taking place at their surface in presence of different environments.

After briefly recalling the basic concepts of FTIR spectrometry, we shall describe the experimental conditions and the specific setups to perform surface analyses. Surface investigations by FTIR spectrometry of silicon nitride, silicon carbide, silicon carbonitride, aluminum nitride and boron nitride nanoparticles will be presented. Comparisons will be made with the surface of the corresponding oxides, thus demonstrating the specificity of the surface composition of these non-oxide materials. Based on infrared experimental results, a model of the surface oxidation of the silicon carbide nanoparticles will be discussed and correlated to *ab initio* calculations.

## Surface Structure and Chemistry of the Boron-Rich Solids

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The techniques used to study solid surfaces have evolved over the past thirty years to the point where the surface structure and surface chemistry of various materials can now be understood on an atomic scale. While the bulk properties of many of the boron-rich solids have been and continue to be the object of many investigations, the surfaces of these materials have received relatively little attention. This is despite the direct relevance of the surface properties to many current and future applications of the boron-rich solids. The history of surface science studies of various boron-rich solids will be reviewed and current work described. The materials that have been studied most extensively are the rare-earth hexaborides, particularly the (100) surface of single-crystals of lanthanum hexaboride. An understanding of the atomic structure of the  $\text{LaB}_6$  (100) surface is required in order to understand why this material has such a low work function. It is the low work function of lanthanum hexaboride that has led to its wide spread use as a high performance thermionic emitter in various electron optical devices. Earlier work on the atomic structure of  $\text{LaB}_6$  (100) as determined by scanning tunneling microscopy (STM) will be described. Recently, STM has been used to study the surface structure of  $\text{YB}_{66}$  (100) and  $\text{HfB}_2$  (0001). A variety of surface sensitive techniques including low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and STM have also been used to study the growth of epitaxial thin films of  $\text{HfB}_2$  on a Hf (0001) single crystal surface.

## Computational Modeling of Surface Layers of Refractory Compounds

E.F.Sheka

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This lecture presents an overview of the modern trends in the surface study provided by quantum-chemical (QCh) approaches split into four parts. Part 1 introduces the fundamental grounds of the QCh approaches in surface description and presents calculation techniques. The main attention is given to advanced semiempirical QCh methods providing quantitative consideration of reasonably large pieces of real surfaces. Part 2 describes quantitative characteristics of surfaces allowed by the approach among which there are Cartesian and internal atom coordinates, charge and spin density distribution over surface atoms, atom Wiberg's indices describing interatomic bonding, and free valency indices disclosing the meaning of surface "dangling bonds". Application of the QCh approach based on AM1 and PM3 semiempirical methods to bare and terminated surfaces of silicon, silicon nitride, silicon carbide, and silicon dioxide is considered in Part 3. Part 4 is related to processes involving species surfaces, such as interface formation provided by both adsorption and interspecies interaction, electric field stimulated graft oligomerisation on and desorption from the surface, as well as crack formation and sliding friction on the surface. A total combination of the presented results gives a clear vision of modern facilities of the QCh approach in studying various processes occurred on surface layers of refractory compounds.

## Numerical Modeling of Surface Reactions

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The use of numerical simulations to study the properties of materials has now grown into a mature field. The exponential increase in computational power of recent decades has made possible the application of advanced numerical approaches, such as time-dependent Monte Carlo and molecular dynamics simulations, and provided the means for investigation of larger and more complex systems. Numerical simulations are well suited to the study of surface reactions and related phenomena. Surface smoothness and texture of deposited films, deposition rate and efficiency, material etching, and formation of nanostructures are just a few familiar examples where knowledge of surface processes is required. While both physical and chemical transformations are of concern, the present discussion is focused on ability to understand and model chemical reactions, i.e., surface transformations that involve making and breaking of molecular bonds. The objective of the present discussion is to review theoretical approaches to study surface reactions, focusing on going from an atomistic level to mesoscale description to macroscale phenomena. The suggested methods include quantum-mechanical calculations of surface models, time-dependent Monte Carlo simulations using reaction probabilities derived from the quantum-mechanical calculations, and kinetic modeling parameterized to the Monte Carlo results. The examples are drawn from the fields of silicon, diamond, and carbon materials, stressing the methodology and emphasizing general features revealed in recent numerical simulations.



**Ternary Metal Boron Carbides: Constitution, Thermodynamics,  
Compound Formation and Structural Chemistry**

Peter Franz Rogl

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Combinations of high hardness borides and boron carbide are attractive materials for a variety of technological high temperature applications. Whether prepared and manufactured under equilibrium or under nonequilibrium conditions, the performance of these composite materials under high temperature abrasive wear conditions will largely depend on the thermodynamic conditions of phase compatibilities and phase equilibria. A simple classification of these ternary systems in terms of four principal types is possible on the basis of the ability of the metal atom M to form binary compounds MB and/or MC and the ability to form ternary compounds. Thermodynamic calculation of the constitutional diagrams has been carried out for the refractory systems with M=Ti,Zr,Hf,V,W providing a consistent set of thermodynamic data to be used in the predictive calculation of higher order systems  $M^1-M^2-\dots M^n-B-C$ .

## **Interfaces in Ceramics**

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This lecture deals with theoretical models of interfaces (intergrain and interphase boundaries) in ceramics with the special attention being paid to non-periodic interfaces in boride, carbide and nitride materials. Geometric and continuum models of such interfaces are considered. The role of interfaces in plastic deformation processes in boride, carbide and nitride materials is discussed.

**Self-Propagating High-Temperature Synthesis of Carbides, Nitrides and Borides**

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Discussed is one of the fast developing branches of materials science, Self-propagating High-temperature Synthesis (SHS) of inorganic compounds and materials. In these processes, synthesis takes place not in the entire charge volume (as in furnace technique) but in a layer that, after local initiation, propagates through a charge in the form of the combustion wave.

General information about SHS processes is presented (burning velocity, combustion temperature, parameters of initiation, structural types of charge, chemical reactions, mechanisms of combustion and structure formation, synthesized products, etc.).

Discussed are the features of SHS related to the gasless and infiltration character of combustion, heterogeneous structure of charge, existence of the homogeneity range, optimization of synthesis conditions, and using the means of control. Examples of synthesized carbides, nitrides, and borides are given along with certification of products obtained under optimized synthesis conditions.

Special attention is given to the main technological types of SHS: (1) chemical synthesis, (2) SHS sintering, (3) forced SHS compaction, (4) SHS metallurgy, (5) SHS welding (joining), and (6) gas-transport SHS. These types of SHS can be used to produce various materials and items (powders, porous items, consolidated and cast materials, items with desired shape and size), to join refractory materials, and to apply coatings. Discussed are also some typical classes of SHS materials (abrasives, hard alloys, ceramics, functionally graded materials, high- $T_c$  superconductors, etc.). Exemplified are the "classical" and new practical applications of SHS.

For this branch of modern materials science, some promising directions of research are outlined.

**Synthesis, Physical and Chemical Properties of Rare Earth Borides**

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The creation of new materials based on refractory compounds of metal and non-metal elements is now an exceptionally important problem. These materials are necessary both for solution of common tasks of modern high temperature techniques and for production of essentially new devices and equipment which use new fundamental physical phenomena.

**Boride/Nitride Composites: Synthesis and Properties**

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In recent years nitride and boride ceramics have been developed due to their specific properties and potential applications. Although every engineering material has a field of application in its pure form, increasing attention has been devoted to composites in which pure components are mixed to give new materials with tailored properties.

The addition of dispersed particles, whiskers or platelets to ceramic matrices has been a common approach to enhancement of mechanical properties such as fracture toughness. However, for many systems the influence is generally small and an alternative reason for this approach is to improve electrical or thermal conductivity in previously insulating ceramics. In the case of an electrically non-conductive ceramic ( $\text{AlN}$ ,  $\text{Si}_3\text{N}_4$ ,  $\beta$ -sialon,  $\text{SiC}$ ...), the addition of a conductive second phase ( $\text{TiN}$ ,  $\text{TiB}_2$ ,  $\text{ZrB}_2$ ,  $\text{TiC}$ ...) may confer sufficient conductivity to allow spark discharge machining and avoid some of the expense of diamond grinding in the preparation of components. The development of such composites has been considered for some specific applications in the field of heaters, igniters, cutting tools, corrosion or wear-resistant parts and complex-shaped structural components. Their properties are strongly influenced by the microstructure and therefore by the starting compositions and the processing parameters.

The aim of this review is to describe the preparation and characterization of boride/nitride composites and discuss the evolution of their mechanical properties and oxidation behaviour as a function of their composition and microstructure.

**Physicochemistry of Precursors for Carbide, Nitride, and Boride Synthesis**

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It is common knowledge that physical-mechanical and physical-chemical properties of powders, bulks, films, and coatings are closely determined by precursors for different methods of synthesis and decomposition. A wide variety of precursors for non-oxide advanced ceramics is considered and discussed. The special attention is given to precursors for materials based both on covalent compounds ( $\text{Si}_3\text{N}_4$ ,  $\text{SiC}$ ,  $\text{BN}$ ,  $\text{B}_4\text{C}$ , and  $\text{AlN}$ ) and on transition metal ones ( $\text{TiN}$ ,  $\text{TiB}_2$ ,  $\text{WC}$ , etc).

**Ceramic Matrix Composites from Polymerorganic Precursors****Selçuk Güçeri**

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The development of preceramic polymers allows the use of established polymer processing techniques such as resin transfer molding to processing ceramic matrix composites. The impregnation of fiber preforms with preceramic polymers or particle-filled preceramic polymers is a complex process involving a large set of thermophysical phenomena. A particular subject of interest is prevention of the particle filtration during impregnation. Using computational approach based on porous media theory and physical methods developed to describe the nonlinear interactions between various processing parameters, a modeling tool can be developed to analyze particle filtration in complex configurations. Compression resin transfer molding can be used as an alternative to conventional resin transfer molding for processing high fiber volume ceramic composites. Computational analysis shows that an important feature of the compression resin transfer molding is an opportunity to achieve a homogeneous particle distribution within the composite through manipulation of the flow path. Composites with a silicon oxycarbide matrix filled with silicon carbide particles and reinforced with Nextel fibers have been developed to illustrate the potential of the suggested computational and experimental approaches.



**Influence of powder treatments methods and additives on sintering, microstructure and properties of nonoxide ceramics**

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The combination of high temperature mechanical, chemical, and physical properties make several non-oxide ceramics useful materials for structural and/or functional applications. Dense materials can often be fabricated only by the use of additives to provide low melting phases which allow liquid phase sintering. However the sintering aids also promote the formation of intergranular phases, which generally limit the high temperature properties, depending on their composition, amount and distribution.

In order to improve the properties or to produce materials with tailored properties, much research is focused on the control of microstructure (grain size and shape, defects, flaws and intergranular phases in terms of amount, distribution and microchemistry) through the production of fine and pure powders, the design of starting composition, and on the development of controlled powder processing and densification procedures.

In the present lecture the influence of starting powder characteristics, of the sintering aids systems and of powder treatment methods are considered and related to sintering behaviour (mainly by hot pressing), microstructure and mechanical (and/or functional) properties. An overview on this matter is presented and examples are shown concerning: some nitrides (silicon nitride, titanium nitride, aluminum nitride), silicon carbide, titanium diboride.

**Deposition, Structure, and Mechanical Properties  
of Nitride-Based Superlattices**

Scott A. Barnett

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In this talk, the deposition, structure, and mechanical properties of transition-metal-nitride-based superlattices are reviewed. Structural characterization techniques specifically useful for superlattices, especially TEM and X-ray diffraction with simulations, are described. Nitride superlattice deposition techniques such as sputtering are discussed and various issues including nucleation, coherency strain relaxation, and ion bombardment effects are described. High-temperature stability of miscible and immiscible superlattices is described. The phenomenon of epitaxial stabilization on non-equilibrium phases is discussed. Mechanical properties of superlattices are described in detail, particularly the large hardness enhancements, e.g. to values exceeding 50 GPa for TiN/NbN superlattices. Mechanical-property models are described.

## Physics of Hardness of High-Melting Compounds

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Refractory compounds may be divided by the electronic structure into two large groups. The first group includes diamond-structure covalent crystals: diamond, SiC, Si<sub>3</sub>N<sub>4</sub>, B<sub>4</sub>C and BN. These crystals are characterized by a spatial tetrahedral distribution of interatomic bonds formed by the overlap of sp<sup>3</sup>-atomic orbitals. The other more numerous group of refractory compounds consists of interstitial solid solutions which form light small atom radius elements with transition metals, carbides, nitrides, oxides, borides and other compounds are formed. The presence of a strong covalent component of interatomic bonds accounts for a high hardness of a number of compounds, for the order and more exceeding hardness of the transition metal used as a basis for the formation of a refractory compound.

The dislocation theory of the temperature dependence of hardness for these materials is presented. The generalized scheme of the temperature dependence of hardness for high-hard materials with high level of Peierls-Nabarro stress is discussed. In these scheme hardness can be determined by three processes:

- by plastic deformation, corresponding to yield stress;
- by phase transformation under pressure, determined by the critical pressure of the phase transformation (typically, of semiconductor-metal type);
- by the processes of brittle fracture, corresponding to the fracture stress of the material.

To characterize the effect of temperature on the mechanical properties of refractory compounds the concept of the characteristic temperature of deformation T\* is presented. T\* is defined as the temperature at which the crystal lattice resistance to the motion of dislocations is essential and causes a sharp growth of flow stress and hardness when the temperature drops below T\*. The modern problems of hardness measurements are discussed. The model of interaction of the rigid indenter with material is presented and on this base the equations for determination by indentation method of hardness from penetration depths, Young's modulus, plasticity characteristic, fracture toughness K<sub>1c</sub> and other mechanical properties are given. Equipment for determination of hardness (including hot and cold hardness) is described.

**Formation of Carbon upon Selective Etching and Decomposition of Carbides**

Y.G. Gogotsi

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It is well known that decomposition of silicon carbide and some other carbides at high temperatures results in the formation of free carbon. Carbon formation can also accompany corrosion and oxidation of carbides. Carbon can be obtained on the surface of carbides by selective etching. A gaseous or liquid etchant (chlorine, supercritical water, etc.) can extract metals from carbides, leaving carbon behind. Our thermodynamic calculations and experimental studies demonstrated the carbon formation on SiC, TiC, WC, TaC, ZrC and other carbides. Some of these processes can be of significant technological importance. For example, this approach can be used to produce carbon coatings on SiC particles, fibers and whiskers. It allows us to solve the problems of uniformity and adherence of coatings, as well as avoid bridging of filaments and/or particles. The principal difference between the described method and other approaches is that the coating is not deposited on the surface of the carbide; rather the carbide surface is converted into carbon. This method can provide a simple and inexpensive route to carbon coatings (thickness from 10 nm to 1-2  $\mu\text{m}$ ) for a wide range of applications. Depending on the carbide substrate and the experimental conditions, dense or porous carbon coatings with a varying  $\text{sp}^2/\text{sp}^3$  carbon ration can be produced.

It is shown that hydrothermal leaching produces a smooth and uniform carbon film on the surface of CVD and polymer-derived SiC fibers, whiskers, platelets and coarse ( $>30\ \mu\text{m}$ ) SiC powders. Similar coatings have been obtained by halogenation of SiC fibers and powders in chlorine-containing environments. Thermodynamic simulation shows that the suggested method can be applied to a variety of carbides, and other halogens can be used as etchants.

**Interaction of Carbides and Nitrides with Halogen Containing Compounds**

Michael McNallan

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SiC, Si<sub>3</sub>N<sub>4</sub> and other silicon based ceramics are generally considered to be resistant to oxidation because they form a protective silica film when exposed to air which limits the rate of the reaction. Silicon halide compounds are volatile at elevated temperatures, however, and silicon reacts rapidly with chlorine without formation of a protective film. In mixed environments containing a halogen, the competition between formation of volatile and condensed products leads to complex reaction kinetics. In chlorine containing mixtures, if the ratio of chlorine to oxygen is low, a protective film forms which reduces the rate of the reaction to that which would be expected in clean air. If the chlorine to oxygen ratio is high enough to produce volatile species, the rate of attack is very rapid, and corrosion products may consist of volatile products and/or silica with a non-protective morphology. The corrosion under these conditions is several orders of magnitude faster than would be expected in clean air. The transition between these regimes of behavior depends on temperature and on the microstructure and sintering aids in the SiC. Silicon nitride is much more resistant to this attack than SiC. The role of other species in the environment, such as hydrogen, on the kinetics of the corrosion will also be discussed.

In addition to direct reactions with the ceramic, volatile halide compounds can also serve to transport other cations to the reacting surface. In particular, alkali metal species strongly accelerate the corrosion of silicon based ceramics by fluxing the normally protective silica scale. In the simultaneous presence of oxygen, halogens, and alkali halide vapors, increasing the partial pressure of the halogen has the effect of decreasing the overall reaction rate by reducing the activity of the alkali species which attack the silica film.

## Interaction of High-Melting Compounds with Aggressive Media

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The refractory compounds and materials on their base find a wide application in a contemporary industry. It is very important to ascertain their high-temperature behaviour under an action of different aggressive media: gas environment, metallic melts, corrosion-active electrolytes. Many fundamental results concerning thermodynamics, kinetics and mechanisms of high-melting compounds interaction with the aggressive media are considered. It was established that the real crystal structure and crystallochemical peculiarities of scale formed, mainly, influence on the kinetics regularities and phase transformations that took place.

In particular, high resistance of AlN as for high-temperature oxidation is explained by formation of dense adherent oxide film because in this case the Pilling-Bedworth ratio is equal to zero. Obviously, due to this reason the possibility of pores, cracks and other film defects formation is excluded. On the contrary, the scale cracking and deterioration of ZrN samples occur because of a nature of phase crystallochemical transformations and intercrystallite character of corrosion cracks development with a further fragmentation of nitride matrix taking place perpendicularly to an oxide layer growth surface. The metals borides are comparatively resistant in oxygen up to 1100 °C. The further rise of temperature significantly increases the oxidation reactions rate. As a rule, the B<sub>2</sub>O<sub>3</sub> being contained in a scale closes the pores and cracks, and the formed borates slow down the diffusion of components through the oxide layers. The essential improvement of corrosion properties, compared with the individual high-melting compounds, has been established for the binary and ternary composite ceramics, in particular, for the AlN-SiC, AlN-ZrB<sub>2</sub>, AlN-TiN, AlN-SiC-ZrB<sub>2</sub> systems. These ceramics have not only extremely high corrosion resistance (sometimes up to 1550 °C), but also the high physicomachanical characteristics, viz., hardness, bending strength, plasticity etc. In a great many cases the formation of intermediate barrier layers plays an essential role in the oxidation process. Herein the high corrosion resistance of such ceramics is, mainly, determined by mullite and borates phases formation.

For the study of kinetics and mechanism of refractory materials high-temperature oxidation the TG, DTA, XRD, SEM, EPMA, metallographic and petrographic analyses methods were used.

The adhesion interaction (kinetics with calculation of wetting energetic parameters) of refractory carbides, borides, and nitrides of metals of IV-VI a groups as well as materials on their base with the liquid metals of I-VIII groups and alloys on their base was studied as well. The regularities of contact interaction of both nonmetallic high-melting compounds (Si<sub>3</sub>N<sub>4</sub>, AlN, SiC, B<sub>4</sub>C) and materials on their base as well as the metal-like refractory compounds with liquid metals of Fe group and their alloys are considered. The analysis of interface interaction from the point of view of thermodynamic characteristics and electrone structure of contacting phases was carried out for the "refractory compound-aggressive metallic melt" systems. The principles of

choice of structural components of composite materials on the base of high-melting compounds with a metallic binder were formulated.

The corrosion properties of high-melting compounds and composites on their base in the aggressive electrolytes (in particular, in sea water) are considered. It was established that the corrosion behaviour of the ceramics is defined by the features of their structure. For instance, the TiN-AlN composite with the equimolar ratio of components which is characterized by a fine-dispersion structure with an uniform distribution of TiN and AlN grains proved to be the most corrosion resistant. The initial stages of these nitride ceramics corrosion are determined by the TiN dissolution with a subsequent formation of  $\text{TiO}_2$  protective film. In the further the AlN interacts with an electrolyte forming  $\text{Al}(\text{OH})_3$  and  $\text{AlO}(\text{OH})$  at the high enough values of anodic potentials. On the surface of TiN:AlN equimolar composite the two-phase protective film containing  $\text{AlO}(\text{OH})$  and  $\text{Na}_4\text{TiO}_4$  titanate formed at the greater values of anodic polarization.

The high-melting compounds and materials on their base can be recommended as high-performance materials for the aggressive media.

NOTES

**Strength and Thermal Shock Resistance of Refractory Compounds**

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General strength dependencies of refractory ceramic materials ( on the examples of carbides ZrC, NbC, ZrC + NbC, SiC, Si<sub>3</sub>N<sub>4</sub> , their compositions with carbon and oxides Al<sub>2</sub>O<sub>3</sub> ,Sc<sub>2</sub>O<sub>3</sub> ,Y<sub>2</sub>O<sub>3</sub> ) are considered in wide temperature range up to 2500 °C in relation to the stress state of samples loaded by tension , bending , torsion or compression. The aspects of plasticity and fracture are regarded on the micro, medium and macro levels. Data on the static, cyclic, long time strength, creep, microhardness and crack propagation are given. Investigation of microstructure revealed deformation peculiarities with variation of grain size and strain conditions. The influence of structural parameters (grain and pore sizes, level of porosity, surface and volume flaws, inclusions) on the strength and fracture are discussed. The statistical parameters of strength dispersion are determined. Methods of thermal and thermal-mechanical treatment (crack healing, quenching, program strengthening) for improving mechanical characteristics of ceramic are considered. Thermal stress resistance (TSR) regularities of porous, dense carbides and compositions with carbon are determined in a wide temperature range up to 2500 °C by the devised test methods. The TSR of ceramics are increased with temperature upgrowth when relaxation of thermal stresses are made possible. The criteria of TSR depending on stress conditions is proposed on the base of fracture mechanics. It is shown that the proper selection of composition and structure can increase the TSR of ceramics up to 2.5 times.



## High Temperature Carbide Structures in Nuclear Energy

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Operating conditions for space nuclear power plants have been considered. High temperatures, radioactive irradiation and neutron physical characteristics of such reactors considerably limit the material choice. Refractory metal carbides are the most suitable for these purposes. In this work main attention paid to thermal strength and radiation stability of the structures made of carbides. The stochastic model to estimate strength of the structures made of brittle materials been suggested. The test results of the main structure elements of nuclear power plants have been presented.

## POSTER PRESENTATIONS

### Poster Session I. Structure and Physical Properties, Modeling

Monday, August 17

Chair: A.I. Gusev

P1-1

Vacancy state in transition carbides and nitrides and its display in Auger spectra

Yu.M.Shulga and V.I.Rubtsov

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P1-2

Two new superconducting phases in Y-Ni-B system

G.Burkhanov<sup>1</sup>, S.Lachenkov<sup>1</sup>, G.Kuz'micheva<sup>2</sup>, and E.Khludov<sup>3</sup>

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<sup>3</sup> International Laboratory of High Magnetic Fields and Low Temperatures, Wroclaw, Poland

P1-3

Structure and physical-mechanical properties of nanostructured TiB<sub>2</sub>/TiN films

R.A.Andrievski<sup>1</sup>, G.V.Kalinnikov<sup>1</sup>, N.Hellgren<sup>2</sup>, P.Sandstrom<sup>2</sup>, and D.V.Shtansky<sup>3</sup>

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<sup>2</sup> Linchoping University, Linchoping, Sweden

<sup>3</sup> Ehime University, Matsuyama, Japan; Russian Scientific Center "Tsniichernet", Moscow, Russia

P1-4

Structural defects of chromium carbide

I.I.Kositsina and V.V.Sagaradze

Institute of Metal Physics, UB of RAS, Ekaterinburg, Russia

P1-5

Deformation and structural peculiarities of nanophase high-melting point compounds

N.I.Noskova<sup>1</sup>, R.A.Andrievski<sup>2</sup>, and V.V.Ivanov<sup>3</sup>

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P1-6

Dynamic compaction of ultrafine TiN powder

R.A.Andrievski<sup>1</sup>, N.I.Noskova<sup>2</sup>, V.V.Ivanov<sup>3</sup>, and E.A.Kozlov<sup>4</sup>

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P1-7

Magnetic susceptibility and short-range order in annealed nonstoichiometric HfC

A.N.Zyryanova and A.I.Gusev

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P1-8

Nitride, oxide, and carbide thin overlayers on Ti(0001): experiment and theory

M.V.Kuznetsov, D.P.Frickel, E.V.Shalaeva, N.I.Medvedeva, and A.V.Tel'nikov

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P1-9

Metastable solid solution of Ti-Si-N(O): synthesis, structure, and stability

E.V.Shalaeva, M.V.Kuznetsov, S.V.Borisov, Medvedeva, and A.I.Gusev

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P1-10

Synthesis and structure of  $Ti_3SiC_2$  carbosilicide

V.V.Karelina, D.G.Kellerman, Ya.N.Blinoskov, and A.I.Gusev

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P1-11

Microplasma noise on structure defects of 6H-SiC

A.M.Svetlichny, V.V.Poljakov, and G.G.Rodnij

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P1-12

Distribution of temperature in SiC substrate by rapid thermal annealing in coherent radiation

O.A.Ageev, A.M.Svetlichny, and D.A.Sechenov

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P1-13

Structure and properties of Ta borides obtained by molten salts electrolysis

E.G.Polyakov, O.V.Makarova, L.P.Polyakova, and A.A.Shevyrov

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P1-14

Magnetic shielding properties of superconducting electrolytic NbC coatings

V.Kolosov and A.Shevyrov

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P1-15

LEDs and multioperated optoelectronic devices based on GaN

V.G.Sidorov<sup>1</sup>, A.G.Drizhuk<sup>2</sup>, D.V.Sidorov<sup>1</sup>, and A.S.Ustinov<sup>3</sup>

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P1-16

Model of self-organized structures in BN

N.A.Sergeev

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P1-17

Modeling of the Surface Oxidation of a Silicon Carbide Nanopowder. An *ab initio* Approach

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P1-18

Modeling interaction of refractory carbides and nitrides with hydrogen and nitrogen

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P1-19

Computer modeling of oxide scale growth on Si<sub>3</sub>N<sub>4</sub> and SiC ceramics

B.A.Galanov<sup>1</sup>, S.M.Ivanov<sup>1</sup>, E.V.Kartuzov<sup>1</sup>, K.G.Nickel<sup>2</sup>, and Yu.G.Gogotsi<sup>3</sup>

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<sup>3</sup> University of Illinois at Chicago, Chicago, USA

P1-20

Raman spectroscopy investigation of disorder and stoichiometry of aluminum-implanted 6H-SiC

V.N. Makarov, A.V. Suvorov

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P1-21

Emission properties of LaB<sub>6</sub>-ZrB<sub>2</sub>-Ni cathodes

A.A.Taran, E.K.Ostrovskiy, and S.S.Ordaniyan

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P1-22

Comparative emission characteristics of composite LaB<sub>6</sub> - and GdB<sub>6</sub>-based cathodes

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P1-23

High temperature thermoionic ZrC-W and ZrC-Mo materials

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P1-24

Using of  $ZrN$  and  $ZrN_xO_y$  as electrodes for vacuum and gas-discharge devices

A.P.Kislitsin, E.K.Ostrovskiy, and S.S.Ordaniyan

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P1-25

Stoichiometric compositions in metallic glasses on the basis of the Fe-B system

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P1-26

New possibilities of  $AlN$  structure and properties development

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<sup>3</sup> University of Technology, Lulea, Sweden

P1-27

Structure and properties of pyrolytic rhombohedral BN

V.I. Rumiantsev, E.V. Toupitsina, A.S. Osmakov, A.E. Kravchik

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P1-28

Some Features of Localized Deformation

M.Yu. Gutkin and I.A. Ovid'ko

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## Poster Session II. Thermal, Physical, Chemical and Mechanical Properties

Tuesday, August 18  
Chair: Yu.V. Mil'man

P2-1

Physico-chemistry, technology and properties of SiC-based materials  
S.S.Ordaniyan  
St.Petersburg State Technological University, St.Petersburg, Russia

P2-2

Arc melting of AlN  
A.V.Kostanovsky, I.A.Zhilyakov, A.V.Kirilin, and L.G.D'achkov  
Scientific Association "Institute of High Temperatures", RAS, Moscow, Russia

P2-3

Oxidation of Mo-S-C-based Composites in Air  
V.P.Kobyakov<sup>1</sup>, G.N.Komratov<sup>1</sup>, V.I.Ponamaryov<sup>1</sup>, V.I.Yukhvid<sup>1</sup>, and  
I.M.Ovchinnikov<sup>2</sup>  
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<sup>2</sup> Institute of Solid State Physics, RAS, Chernogolovka, Russia

P2-4

Thermogravimetric investigation of oxidation of powders of boron-containing composites  
I.B. Ban'kovskaya, B.Z. Pevzner, G.N. Gorbatova  
Institute of Silicate Chemistry, RAS, St.Petersburg, Russia

P2-5

Heat capacity, root-mean-square amplitudes of vibration, and cell parameters of DyB<sub>6</sub> in  
the range 5-300 K  
N.N.Sirota<sup>1</sup> and V.V.Novikov<sup>2</sup>  
<sup>1</sup> Moscow State University of Environmental Engineering, Moscow, Russia  
<sup>2</sup> Bryansk State Pedagogical University, Bryansk, Russia

P2-6

Hydrogen and ammonia interaction with carbide and boride candidate materials for space  
solar heat storage at temperatures above 2000 K  
N.U.Kalashnikov, V.I.Mitrofanov, and V.N.Zagryazkin  
Research Institute "Luch", Podol'sk, Russia

P2-7

Effect of Y<sub>2</sub>O<sub>3</sub> on C+Si<sub>3</sub>N<sub>4</sub> interaction at high temperatures  
A.Kopan  
I.N.Frantsevich Institute for problems of Materials Science, NASU, Kiev, Ukraine

P2-8

Refractory carbide coatings on Nicalon and carbon fibers and their oxidation resistance

N.I.Baklanova, V.N.Kulyukin, M.A.Korchagin, and N.Z.Lyakhov

Institute of Solid State Chemistry and Mechanochemistry, SB of RUS, Novosibirsk, Russia

P2-9

Kinetic and chemical features of TiC powder oxidation

S.F.Korablev

National Technical University, Kiev, Ukraine

P2-10

High-temperature oxidation resistance of high-dense SiC, Si<sub>3</sub>N<sub>4</sub> and AlN specimens

I.R.Korableva<sup>1</sup> and S.F.Korablev<sup>2</sup>

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<sup>2</sup> National Technical University, Kiev, Ukraine

P2-11

Corrosion stability and electrocatalytic activity of some transition carbides and nitrides

T.A.Lukashenko<sup>1</sup>, K.I.Tikhonov<sup>1</sup>, and E.M.Sher<sup>2</sup>

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P2-12

Formation, microstructure and development of localized shear deformation at high temperatures

N.P.Skvortsova

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P2-13

Structure and properties of SiC-TiB<sub>2</sub> ceramics

O.N.Grigoriev<sup>1</sup>, Yu.G.Gogotsi<sup>2</sup>, G.A. Gogotsi<sup>3</sup>, and V.Subbotin<sup>1</sup>

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P2-14

Carbide phase formation under laser-ultrasonic Ti alloying of steel

D.M.Gurreyev, N.N.Kruzhkov, and E.A.Namestnikova

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P2-15

Effect of complex ion-vacuum modification on tribology change of hard alloys

K.N.Poleschenko, G.I.Gering, V.I.Voloshina, S.N.Povoroznjuk, G.A.Vershinin, and

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P2-16

High hardness ceramics for cutting tools based on cubic BN

Yu.A. Alexeev, T.Yu. Tchemekova, Yu.S. Polyahovsky, O.G. Francusov

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P2-17

New tool WC-based materials

I.B.Panteleev and S.S.Ordaniyan

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P2-18

Characterisation of Microstructural Features using High Frequency Ultrasonics

P. Palanichami

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P2-19

Stabilization of light-emitting properties of porous silicon by the high-temperature carbonization

B.M. Kostishko, Sh.R. Atazhanov, S.N. Mikov, I.P. Puzov, A.N. Komov, L.V. Koltsova

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P2-20

Structure and mechanical properties of polycrystalline CrN/TiN superlattices

P. Yashar, K. Martin, S. A. Barnett

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### Poster Session III. Processing, Applications

Wednesday, August 19

Chair: S.Yu. Sharivker

P3-1

Kinetics of sintering of aluminium nitride

U.D. Afonin, U.P. Zaykov

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P3-2

Ultrafine nitride powder as a base for ceramics

E.K. Stepanenko and S.S. Ordaniyan

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P3-3

Consolidation of ultrafine TiN and TiB<sub>2</sub> powders under high pressures and high temperatures

R.A. Andrievski<sup>1</sup>, V.S. Urbanovich<sup>2</sup>, Y. Ogino<sup>3</sup>, T. Yamasaki<sup>3</sup>, and K.Y. Yanushkevich<sup>2</sup>

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<sup>3</sup> Himeji Institute of Technology, Himeji, Japan

P3-4

Properties of refractory metals boride and carbide coatings deposited by electrochemical synthesis from molten salts

S.V. Devyatkin<sup>1</sup>, S.A. Kuznetsov<sup>2</sup>, and V.V. Malyshev<sup>1</sup>

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P3-5

Polydimethylsilathyne as a precursor for SiC

N.I. Baklanova, V.N. Kulyukin, N.Z. Lyakhov, O.G. Yarosh, and M.G. Voronkov

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P3-6

SHS TiC-based materials obtained in artificial gravity conditions

V.N. Sanin

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P3-7

Combustion synthesis of composite SIALON ceramics

K.L. Smirnov and I.P. Borovinskaya

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P3-8

Self-propagating, high-temperature synthesis and structure formation of composite materials of ternary Ti-Si-C, Ti-Si-N and Ti-B-N systems

H.E.Grigoryan<sup>1</sup>, A.E.Rogachev<sup>1</sup>, A.E.Sychev<sup>1</sup>, and E.A.Levashov<sup>2</sup>

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P3-9

Preparation of TiC and TiB<sub>2</sub> specimens by SHS for single crystal growth by plasma-arc melting

M.A.Ponomarev and Yu.A.Sapronov

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P3-10

Plasma-arc melting growth stabilization for refractory single crystal preparation from SHS products

M.A.Ponomarev and Ya.A.Sapronov

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P3-11

Preparation of W-W<sub>2</sub>C alloys by SHS method from WO<sub>3</sub>+C+Al mixes

A.N.Avramchik, N.H.Galchenko, O.K.Lepakova, and O.A.Shkoda

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P3-12

Features of structure formation of SHS alloys in magnetic field

V.D.Kitler, A.I.Kirdjashin, Yu.M.Maximov, O.K.Lepakova, and V.V.Burkin

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P3-13

Nitride synthesis by wire electrical explosion with use of air N<sub>2</sub>

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P3-14

Feature of carbides, nitrides, and borides prepared by wire electrical explosion

V.Ya.Ushakov, A.P.Ilyin, O.B.Nazarenko, D.V.Tikhonov

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P3-15

Synthesis of TiC-WC solution in hydrogen containing equilibrium amount of methane

I.V.Yepik, V.P.Bondarenko, and S.F.Korablev

V.N.Bakul' Institute for Superhard Materials, NASU, Kiev, Ukraine

P3-16

Role of ultrafine powders in the formation of single-phase materials (on the example of Ti carbonitride)

I.Ivanov<sup>1</sup>, S.Ordaniyan<sup>1</sup>, L.Mashulia<sup>1</sup>, and I.Zalite<sup>2</sup>

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P3-17

New technology of composite powder for functional ceramics

Yu.P.Udalov, S.S.Ordaniyan, G.S.Safronova, O.N.Kovaleva, and Yu.L.Sidorovsky

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P3-18

Titanium carbide, nitride and carbide/nitride processing by metalthermal halogenide reduction

S.V.Aleksandrovsky, V.N.Sizyakov, and A.H.Ratner

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P3-19

Currentless TaC film formation in molten salts

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P3-20

Mechanochemical synthesis of nanophase refractory carbides

M.Savyak, I.Uvarova, I.Timofeeva, L.Isayeva, and S.Kirilenko

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P3-21

WC-based ceramic material synthesis by crystallization of amorphous solid solution

E.Yu.Belyaev, G.A.Suchkova, and O.I.Lomovsky

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P3-22

Investigation and elaboration of gas-thermal synthesis of specific powder materials

V.A.Artyukhov, A.Yu.Bord, and V.K.Sheleg

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P3-23

Carbon (graphite) interfaces in tribological materials

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P3-24

Fabrication of Dense SiC and  $\alpha$ -Si<sub>3</sub>N<sub>4</sub> Ceramics Under High Static Pressures

V.S.Urbanovich<sup>1</sup>, K.G.Nickel<sup>2</sup>, Y.G.Gogotsi<sup>3</sup>, M.Backhaus-Ricoult<sup>4</sup>,  
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P3-25

Composites with a ceramic matrix

V.V. Kartashov, V.A. Yazev, A.R. Beketov

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P3-26

Ceramic materials based on Si<sub>3</sub>N<sub>4</sub>-TiN from ultra-high dispersion powders

L.L. Sartinska, I.I. Osipova, A.M. Koval'chenko

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P3-27

The effect of explosive shock treatment on the formation of nitrides in a Ti-6Al-4V alloy

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P3-28

Mechanosynthesis of iron carbides at composition Fe<sub>75</sub>C<sub>25</sub>

F. Miani

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P3-29

Combining Materials Science Principles for the Optimization of Metal/Nitride Bonding

O. Paiva, M.A. Barbosa

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P3-30

Formation of Transition Metal Nitride Films by Rapid Thermal Processing

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